



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:17 PM GMT

PDB ID : 1XPL
Title : Crystal Structure of Staphylococcus aureus HMG-COA Synthase with Acetoacetyl-COA and Acetylated Cysteine
Authors : Theisen, M.J.; Misra, I.; Saadat, D.; Campobasso, N.; Miziorko, H.M.; Harrison, D.H.T.
Deposited on : 2004-10-08
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

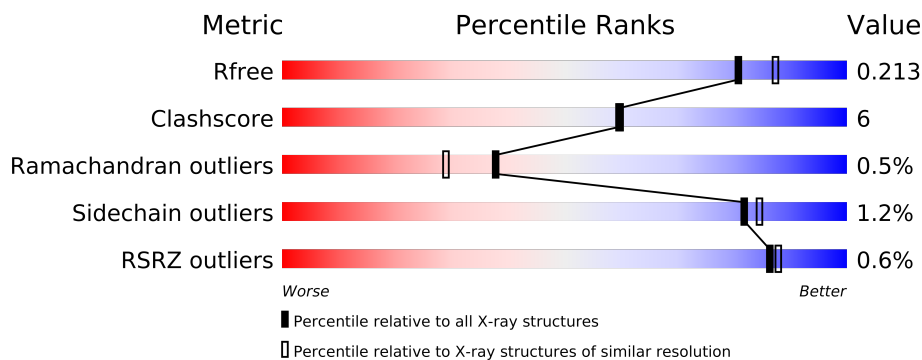
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12654 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxy-3-methylglutarylCoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	4	0
			2979	1905	501	562	11			
1	B	389	Total	C	N	O	S	0	4	0
			2973	1904	500	558	11			
1	C	389	Total	C	N	O	S	0	7	0
			3005	1922	505	567	11			
1	D	389	Total	C	N	O	S	0	4	0
			2986	1911	504	560	11			

There are 44 discrepancies between the modelled and reference sequences:

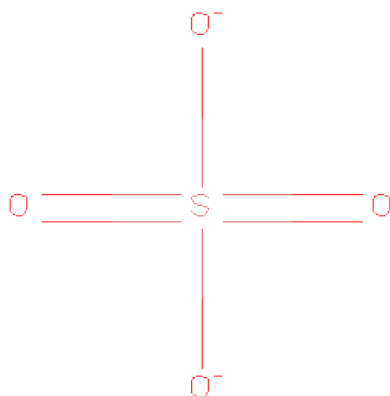
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
A	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
A	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
A	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
A	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
A	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
B	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
B	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
B	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
B	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
B	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6

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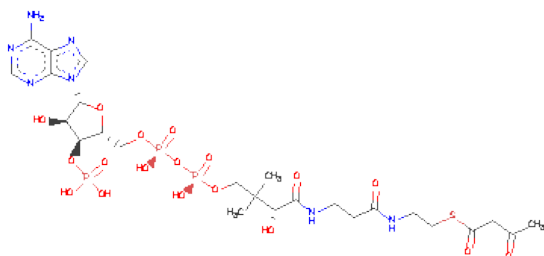
Chain	Residue	Modelled	Actual	Comment	Reference
B	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
C	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
C	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
C	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
C	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
C	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
D	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
D	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
D	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
D	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
D	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 54 25 7 18 3 1	0	0
3	B	1	Total C N O P S 54 25 7 18 3 1	0	0
3	C	1	Total C N O P S 54 25 7 18 3 1	0	0
3	D	1	Total C N O P S 54 25 7 18 3 1	0	0

- Molecule 4 is water.

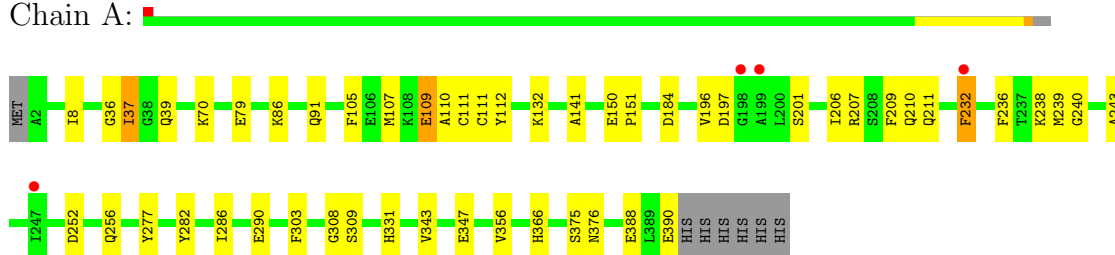
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total 113	O 113	0	0
4	B	121	Total 121	O 121	0	0
4	C	119	Total 119	O 119	0	1
4	D	102	Total 102	O 102	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

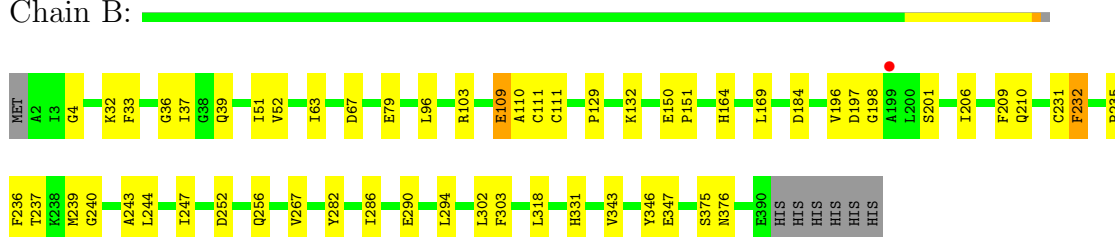
- Molecule 1: 3-hydroxy-3-methylglutarylCoA synthase

Chain A:



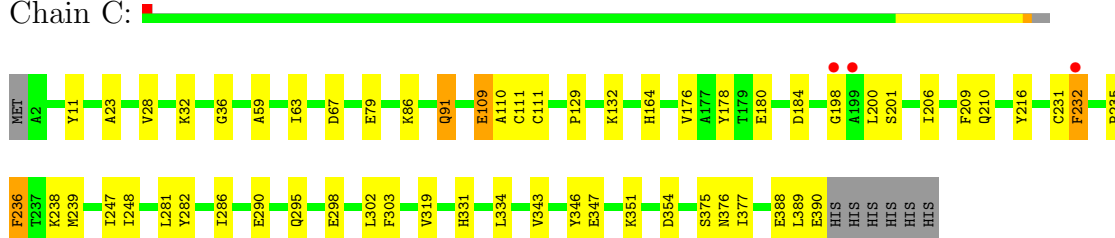
- Molecule 1: 3-hydroxy-3-methylglutarylCoA synthase

Chain B:



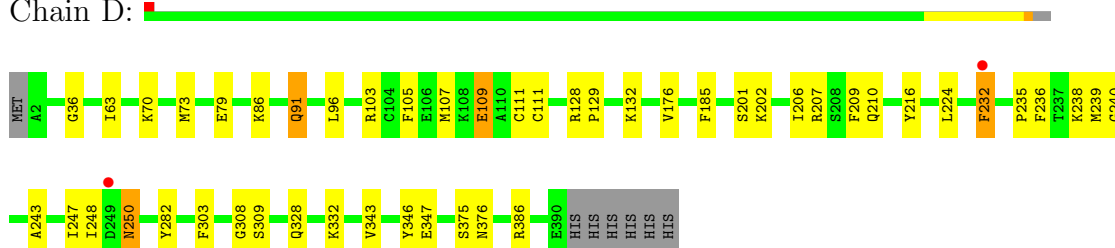
- Molecule 1: 3-hydroxy-3-methylglutarylCoA synthase

Chain C:



- Molecule 1: 3-hydroxy-3-methylglutarylCoA synthase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.33Å 118.41Å 121.63Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	29.50 – 2.00 29.45 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.50-2.00) 86.1 (29.45-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.234 0.196 , 0.213	Depositor DCC
R_{free} test set	5269 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.1	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.467 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 105323 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12654	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8286e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAA, SCY, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3038	0.57	0/4128
1	B	0.34	0/3032	0.58	0/4121
1	C	0.34	0/3066	0.59	0/4169
1	D	0.33	0/3043	0.59	0/4130
All	All	0.33	0/12179	0.58	0/16548

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	TYR	Sidechain
1	B	282	TYR	Sidechain
1	C	282	TYR	Sidechain
1	D	282	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2979	0	2820	32	0
1	B	2973	0	2811	33	0
1	C	3005	0	2842	41	0
1	D	2986	0	2840	35	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	54	0	36	0	0
3	B	54	0	36	4	0
3	C	54	0	36	3	0
3	D	54	0	36	1	0
4	A	113	0	0	1	0
4	B	121	0	0	1	0
4	C	119	0	0	1	0
4	D	102	0	0	0	0
All	All	12654	0	11457	141	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (141) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:201:SER:O	1:D:201:SER:CA	1.82	1.27
1:D:201:SER:CA	1:D:202:LYS:N	2.20	1.04
1:C:235[B]:PRO:HG3	3:C:3401:CAA:H22	1.44	0.99
1:D:201:SER:O	1:D:202:LYS:N	1.96	0.99
1:C:36:GLY:O	1:C:238:LYS:HG3	1.83	0.77
1:D:79:GLU:OE2	1:D:111[A]:SCY:HE2	1.93	0.69
1:B:235:PRO:HG3	3:B:2401:CAA:H22	1.75	0.69
1:A:36:GLY:O	1:A:238:LYS:HG3	1.95	0.67
1:A:79:GLU:OE2	1:A:111[A]:SCY:HE2	1.95	0.66
1:A:111[A]:SCY:H	1:A:111[A]:SCY:CD	2.10	0.65
1:A:232[B]:PHE:HB3	1:A:303:PHE:HB3	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:232[B]:PHE:HE1	1:D:240:GLY:CA	2.12	0.62
1:D:232[A]:PHE:CD1	1:D:232[A]:PHE:N	2.68	0.62
1:A:232[A]:PHE:CD1	1:A:232[A]:PHE:N	2.69	0.61
1:D:206:ILE:O	1:D:210:GLN:HG3	2.01	0.61
1:D:232[B]:PHE:HB3	1:D:303:PHE:HB3	1.85	0.59
1:C:111[A]:SCY:CD	1:C:111[A]:SCY:H	2.16	0.58
1:C:86:LYS:HE2	1:C:91:GLN:OE1	2.03	0.58
1:B:343:VAL:O	1:B:347:GLU:HG3	2.03	0.58
1:D:328:GLN:O	1:D:332:LYS:HG2	2.04	0.58
1:A:206:ILE:O	1:A:210:GLN:HG3	2.03	0.58
1:B:110:ALA:HB1	1:B:111[A]:SCY:OCD	2.03	0.58
1:A:196:VAL:HG12	1:A:197:ASP:N	2.19	0.57
1:A:105:PHE:HE1	1:A:107:MET:HE2	1.69	0.57
1:C:236:PHE:CZ	1:C:239:MET:HB2	2.41	0.56
1:B:236:PHE:CZ	1:B:239:MET:HB2	2.40	0.56
1:A:70:LYS:CE	1:A:132:LYS:HE2	2.36	0.56
1:D:111[A]:SCY:H	1:D:111[A]:SCY:CD	2.19	0.55
1:C:235[B]:PRO:HD2	1:C:239:MET:HG2	1.88	0.55
1:B:252:ASP:O	1:B:256:GLN:HG3	2.06	0.55
1:C:232[B]:PHE:HB3	1:C:303:PHE:HB3	1.88	0.55
1:B:111[A]:SCY:HE3	3:B:2401:CAA:O3	2.07	0.54
1:C:206:ILE:O	1:C:210:GLN:HG3	2.07	0.54
1:C:111[A]:SCY:HE3	3:C:3401:CAA:O3	2.07	0.54
1:C:235[A]:PRO:HG3	1:C:239:MET:HG2	1.90	0.53
1:C:110:ALA:HB1	1:C:111[A]:SCY:OCD	2.08	0.53
1:C:286:ILE:O	1:C:290:GLU:HG3	2.08	0.53
1:A:232[B]:PHE:HE1	1:A:240:GLY:CA	2.21	0.53
1:D:375:SER:O	1:D:376:ASN:HB2	2.08	0.53
1:A:375:SER:O	1:A:376:ASN:HB2	2.09	0.53
1:A:209[B]:PHE:HD1	1:A:243:ALA:HB1	1.74	0.52
1:A:343:VAL:O	1:A:347:GLU:HG3	2.09	0.52
1:B:209[A]:PHE:CZ	1:B:247:ILE:HD12	2.44	0.52
1:A:252:ASP:O	1:A:256:GLN:HG3	2.10	0.52
1:D:232[B]:PHE:HE1	1:D:240:GLY:HA3	1.75	0.52
1:B:286:ILE:O	1:B:290:GLU:HG3	2.09	0.52
1:B:129:PRO:HA	1:B:164:HIS:CD2	2.45	0.52
1:C:129:PRO:HA	1:C:164:HIS:CD2	2.45	0.51
1:C:198:GLY:C	1:C:200:LEU:H	2.13	0.51
3:B:2401:CAA:HN8	3:B:2401:CAA:H141	1.75	0.51
1:C:232[A]:PHE:N	1:C:232[A]:PHE:CD1	2.78	0.51
1:B:206:ILE:O	1:B:210:GLN:HG3	2.11	0.50
1:B:237:THR:HG22	1:B:267:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:63:ILE:HD11	1:D:96:LEU:HD22	1.94	0.50
1:D:224:LEU:HD13	1:D:248:ILE:HG22	1.94	0.49
1:C:247:ILE:HG13	1:C:248:ILE:N	2.28	0.49
1:D:386:ARG:HG3	1:D:386:ARG:HH11	1.78	0.48
1:D:343:VAL:O	1:D:347:GLU:HG3	2.14	0.48
1:D:235:PRO:HG3	1:D:239:MET:HG2	1.95	0.48
1:A:366:HIS:HB3	4:A:1576:HOH:O	2.13	0.48
1:A:184:ASP:HB2	1:A:201:SER:HA	1.96	0.48
1:B:184:ASP:HB2	1:B:201:SER:HA	1.96	0.48
1:B:67:ASP:OD1	1:B:132:LYS:HE3	2.14	0.47
1:C:184:ASP:HB2	1:C:201:SER:HA	1.97	0.47
1:C:198:GLY:O	1:C:200:LEU:N	2.46	0.47
1:A:141:ALA:HA	1:A:277:TYR:CE2	2.49	0.47
1:B:244:LEU:O	1:B:247:ILE:HG22	2.14	0.47
1:D:176:VAL:CG1	1:D:216:TYR:HB2	2.45	0.47
1:B:32:LYS:O	1:B:36:GLY:HA3	2.14	0.47
1:B:375:SER:O	1:B:376:ASN:HB2	2.14	0.47
1:D:91:GLN:HE21	1:D:91:GLN:HB2	1.63	0.46
1:D:209[A]:PHE:CZ	1:D:247:ILE:HD13	2.50	0.46
1:A:236:PHE:CZ	1:A:239:MET:HB2	2.50	0.46
1:D:176:VAL:HG11	1:D:216:TYR:HB2	1.97	0.46
1:A:8:ILE:HG12	1:A:286:ILE:HD11	1.97	0.46
1:C:79:GLU:OE2	1:C:111[A]:SCY:HE2	2.16	0.46
1:C:375:SER:O	1:C:376:ASN:HB2	2.16	0.46
1:C:32:LYS:O	1:C:36:GLY:HA3	2.16	0.45
1:B:232[A]:PHE:CD1	1:B:232[A]:PHE:N	2.84	0.45
1:D:248:ILE:C	1:D:250:ASN:H	2.20	0.45
1:D:86:LYS:HE2	1:D:91:GLN:OE1	2.17	0.45
1:A:86:LYS:HE2	1:A:91:GLN:OE1	2.16	0.45
1:C:209[A]:PHE:HE2	1:C:247:ILE:HG12	1.81	0.45
1:C:388:GLU:C	1:C:390:GLU:H	2.20	0.45
1:B:33:PHE:O	1:B:37:ILE:HG12	2.17	0.45
1:A:209[B]:PHE:CD1	1:A:243:ALA:HB1	2.51	0.45
1:B:209[B]:PHE:HD1	1:B:243:ALA:HB1	1.82	0.45
1:D:207:ARG:HG3	1:D:207:ARG:HH11	1.81	0.45
1:D:105:PHE:HE1	1:D:107:MET:HE2	1.82	0.44
1:B:196:VAL:HG12	1:B:197:ASP:N	2.31	0.44
1:B:232[B]:PHE:HE1	1:B:240:GLY:CA	2.29	0.44
1:C:209[A]:PHE:CZ	1:C:247:ILE:HD13	2.53	0.44
1:D:70:LYS:CE	1:D:132:LYS:HE3	2.48	0.44
1:B:150:GLU:HB3	1:B:151:PRO:HD3	1.99	0.43
1:D:308:GLY:N	1:D:309:SER:HA	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:GLY:N	1:A:309:SER:HA	2.33	0.43
1:A:388:GLU:C	1:A:390:GLU:H	2.22	0.43
1:C:67:ASP:OD1	1:C:132:LYS:HE3	2.19	0.43
1:C:343:VAL:O	1:C:347:GLU:HG3	2.18	0.43
1:A:110:ALA:HB1	1:A:111[A]:SCY:OCD	2.19	0.43
1:D:73:MET:HG2	1:D:103:ARG:HB2	2.01	0.43
1:B:294:LEU:HB2	1:B:318:LEU:HD11	1.99	0.43
1:D:209[B]:PHE:HD1	1:D:243:ALA:HB1	1.83	0.43
1:B:232[B]:PHE:HB3	1:B:303:PHE:HB3	2.00	0.43
1:B:111[A]:SCY:HE3	3:B:2401:CAA:C3	2.48	0.43
1:B:79:GLU:OE2	1:B:111[A]:SCY:HE2	2.18	0.43
1:A:232[B]:PHE:HE1	1:A:240:GLY:HA3	1.83	0.43
1:B:290:GLU:OE2	1:B:331:HIS:ND1	2.51	0.43
1:D:236:PHE:CZ	1:D:239:MET:HB2	2.53	0.43
1:D:201:SER:O	1:D:202:LYS:CA	2.66	0.42
1:B:39:GLN:HB3	4:B:2531:HOH:O	2.17	0.42
1:A:112:TYR:OH	1:B:103:ARG:HG2	2.19	0.42
1:C:59:ALA:O	1:C:63:ILE:HG12	2.20	0.42
1:B:63:ILE:HD11	1:B:96:LEU:HD22	2.00	0.42
1:C:178:TYR:CZ	1:C:180:GLU:HG3	2.54	0.42
1:A:207:ARG:O	1:A:211:GLN:HG2	2.19	0.42
1:D:36:GLY:O	1:D:238:LYS:HG2	2.19	0.42
1:C:290:GLU:OE2	1:C:331:HIS:ND1	2.52	0.42
1:C:232[B]:PHE:CB	1:C:303:PHE:HB3	2.49	0.41
1:C:176:VAL:CG1	1:C:216:TYR:HB2	2.50	0.41
1:C:11:TYR:HA	1:C:334:LEU:HD21	2.02	0.41
1:D:185:PHE:C	1:D:185:PHE:CD1	2.93	0.41
1:A:290:GLU:OE2	1:A:331:HIS:ND1	2.53	0.41
1:D:128:ARG:HA	1:D:129:PRO:HD2	1.89	0.41
1:C:319:VAL:HA	4:C:3595:HOH:O	2.20	0.41
1:C:295:GLN:HB2	1:C:298:GLU:HG3	2.02	0.41
1:C:351:LYS:HA	1:C:354:ASP:OD2	2.21	0.41
1:C:111[A]:SCY:HE3	3:C:3401:CAA:C3	2.51	0.41
1:A:196:VAL:CG1	1:A:197:ASP:N	2.84	0.41
1:D:36:GLY:HA3	3:D:4401:CAA:O4B	2.21	0.41
1:A:150:GLU:HB3	1:A:151:PRO:HD3	2.03	0.41
1:A:37:ILE:HG13	1:A:39:GLN:HG2	2.02	0.41
1:B:51:ILE:HG13	1:B:52:VAL:N	2.36	0.41
1:C:235[B]:PRO:HG2	1:C:236:PHE:CD1	2.56	0.40
1:C:232[B]:PHE:HA	1:C:281:LEU:HD13	2.02	0.40
1:B:231:CYS:O	1:B:302:LEU:HA	2.21	0.40
1:A:356:VAL:HG12	1:A:356:VAL:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:376:ASN:CG	1:C:377:ILE:N	2.75	0.40
1:B:4:GLY:HA3	1:B:169:LEU:O	2.21	0.40
1:C:23:ALA:HB1	1:C:28:VAL:HG23	2.02	0.40
1:C:231:CYS:O	1:C:302:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/397 (98%)	367 (94%)	21 (5%)	1 (0%)	50	44
1	B	389/397 (98%)	372 (96%)	15 (4%)	2 (0%)	38	29
1	C	392/397 (99%)	373 (95%)	16 (4%)	3 (1%)	27	17
1	D	387/397 (98%)	366 (95%)	19 (5%)	2 (0%)	38	29
All	All	1557/1588 (98%)	1478 (95%)	71 (5%)	8 (0%)	38	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	B	109	GLU
1	C	109	GLU
1	C	236	PHE
1	C	389	LEU
1	D	109	GLU
1	D	250	ASN
1	B	198	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of

similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/326 (88%)	284 (99%)	4 (1%)	78	81
1	B	285/326 (87%)	281 (99%)	4 (1%)	78	81
1	C	292/326 (90%)	287 (98%)	5 (2%)	73	75
1	D	289/326 (89%)	284 (98%)	5 (2%)	73	75
All	All	1154/1304 (88%)	1136 (98%)	18 (2%)	82	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	109	GLU
1	A	232[A]	PHE
1	A	232[B]	PHE
1	B	109	GLU
1	B	232[A]	PHE
1	B	232[B]	PHE
1	B	346	TYR
1	C	91	GLN
1	C	109	GLU
1	C	232[A]	PHE
1	C	232[B]	PHE
1	C	346	TYR
1	D	91	GLN
1	D	109	GLU
1	D	232[A]	PHE
1	D	232[B]	PHE
1	D	346	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	325	HIS
1	B	325	HIS
1	C	325	HIS
1	D	325	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	SCY	A	111[A]	1	8,8,9	6.51	2 (25%)	7,9,11	1.48	1 (14%)
1	SCY	B	111[A]	1	8,8,9	6.26	2 (25%)	7,9,11	1.21	1 (14%)
1	SCY	C	111[A]	1	8,8,9	6.12	2 (25%)	7,9,11	1.32	1 (14%)
1	SCY	D	111[A]	1	8,8,9	6.28	2 (25%)	7,9,11	1.32	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	A	111[A]	1	-	2/5/7/9	0/0/0/0
1	SCY	B	111[A]	1	-	2/5/7/9	0/0/0/0
1	SCY	C	111[A]	1	-	2/5/7/9	0/0/0/0
1	SCY	D	111[A]	1	-	2/5/7/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	SCY	O-C	18.12	1.23	1.11
1	D	111[A]	SCY	O-C	17.43	1.23	1.11
1	B	111[A]	SCY	O-C	17.43	1.23	1.11
1	C	111[A]	SCY	O-C	17.03	1.23	1.11
1	D	111[A]	SCY	CA-C	2.92	1.53	1.48
1	A	111[A]	SCY	CA-C	2.88	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111[A]	SCY	CA-C	2.72	1.53	1.48
1	B	111[A]	SCY	CA-C	2.54	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111[A]	SCY	CB-SG-CD	-2.66	99.08	100.97
1	B	111[A]	SCY	CB-SG-CD	-2.24	99.38	100.97
1	D	111[A]	SCY	CB-SG-CD	2.13	102.48	100.97
1	A	111[A]	SCY	CB-SG-CD	2.10	102.46	100.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	111[A]	SCY	CE-CD-SG-CB
1	D	111[A]	SCY	OCD-CD-SG-CB
1	A	111[A]	SCY	CE-CD-SG-CB
1	A	111[A]	SCY	OCD-CD-SG-CB
1	C	111[A]	SCY	CE-CD-SG-CB
1	B	111[A]	SCY	CE-CD-SG-CB
1	C	111[A]	SCY	OCD-CD-SG-CB
1	B	111[A]	SCY	OCD-CD-SG-CB

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CAA	A	1401	-	56,56,56	0.81	1 (1%)	83,83,83	1.27	4 (4%)
2	SO4	A	1501	-	4,4,4	0.52	0	6,6,6	13.15	1 (16%)
2	SO4	A	1502	-	4,4,4	0.83	0	6,6,6	12.95	1 (16%)
3	CAA	B	2401	-	56,56,56	0.80	1 (1%)	83,83,83	1.28	4 (4%)
2	SO4	B	2501	-	4,4,4	0.79	0	6,6,6	13.20	1 (16%)
2	SO4	B	2502	-	4,4,4	0.24	0	6,6,6	13.17	1 (16%)
3	CAA	C	3401	-	56,56,56	0.78	0	83,83,83	1.32	4 (4%)
2	SO4	C	3501	-	4,4,4	0.96	0	6,6,6	12.71	1 (16%)
2	SO4	C	3502	-	4,4,4	0.89	0	6,6,6	12.84	1 (16%)
3	CAA	D	4401	-	56,56,56	0.78	3 (5%)	83,83,83	1.29	4 (4%)
2	SO4	D	4501	-	4,4,4	1.59	1 (25%)	6,6,6	12.35	1 (16%)
2	SO4	D	4502	-	4,4,4	1.25	1 (25%)	6,6,6	12.95	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAA	A	1401	-	-	0/55/71/71	0/1/3/3
2	SO4	A	1501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1502	-	-	0/0/0/0	0/0/0/0
3	CAA	B	2401	-	-	0/55/71/71	0/1/3/3
2	SO4	B	2501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2502	-	-	0/0/0/0	0/0/0/0
3	CAA	C	3401	-	-	0/55/71/71	0/1/3/3
2	SO4	C	3501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3502	-	-	0/0/0/0	0/0/0/0
3	CAA	D	4401	-	-	0/55/71/71	0/1/3/3
2	SO4	D	4501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4502	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4501	SO4	O2-S	3.16	1.57	1.47
3	A	1401	CAA	C1-S1P	2.56	1.81	1.76
2	D	4502	SO4	O2-S	2.47	1.55	1.47
3	B	2401	CAA	C1-S1P	2.41	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4401	CAA	C1-S1P	2.05	1.80	1.76
3	D	4401	CAA	P1A-O3A	2.01	1.63	1.59
3	D	4401	CAA	P2A-O3A	2.00	1.63	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2501	SO4	O2-S-O1	-32.34	2.56	109.53
2	B	2502	SO4	O2-S-O1	-32.26	2.81	109.53
2	A	1501	SO4	O2-S-O1	-32.20	3.02	109.53
2	D	4502	SO4	O2-S-O1	-31.72	4.59	109.53
2	A	1502	SO4	O2-S-O1	-31.72	4.59	109.53
2	C	3502	SO4	O2-S-O1	-31.44	5.51	109.53
2	C	3501	SO4	O2-S-O1	-31.12	6.57	109.53
2	D	4501	SO4	O2-S-O1	-30.24	9.51	109.53
3	B	2401	CAA	P2A-O3A-P1A	-7.61	109.38	131.68
3	A	1401	CAA	P2A-O3A-P1A	-7.55	109.54	131.68
3	C	3401	CAA	P2A-O3A-P1A	-7.36	110.10	131.68
3	D	4401	CAA	P2A-O3A-P1A	-7.24	110.44	131.68
3	C	3401	CAA	C2-C1-S1P	-6.20	106.71	113.43
3	D	4401	CAA	C2-C1-S1P	-5.78	107.17	113.43
3	B	2401	CAA	C2-C1-S1P	-5.61	107.35	113.43
3	A	1401	CAA	C2-C1-S1P	-5.51	107.46	113.43
3	C	3401	CAA	O1-C1-S1P	3.62	126.66	122.85
3	D	4401	CAA	O1-C1-S1P	3.34	126.37	122.85
3	B	2401	CAA	O1-C1-S1P	3.29	126.32	122.85
3	A	1401	CAA	O1-C1-S1P	3.13	126.14	122.85
3	C	3401	CAA	O1-C1-C2	2.48	126.62	122.75
3	D	4401	CAA	O1-C1-C2	2.37	126.46	122.75
3	A	1401	CAA	O1-C1-C2	2.33	126.40	122.75
3	B	2401	CAA	O1-C1-C2	2.29	126.33	122.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/397 (98%)	-0.12	4 (1%) 79 80	9, 21, 35, 48	2 (0%)
1	B	390/397 (98%)	-0.16	1 (0%) 91 93	9, 21, 35, 44	2 (0%)
1	C	390/397 (98%)	-0.15	3 (0%) 83 84	8, 21, 35, 46	2 (0%)
1	D	390/397 (98%)	-0.12	2 (0%) 88 89	9, 21, 35, 50	2 (0%)
All	All	1560/1588 (98%)	-0.14	10 (0%) 86 88	8, 21, 35, 50	8 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	GLY	3.4
1	B	199	ALA	3.3
1	C	199	ALA	2.9
1	A	232[A]	PHE	2.5
1	D	232[A]	PHE	2.5
1	D	249	ASP	2.3
1	A	199	ALA	2.2
1	C	232[A]	PHE	2.1
1	A	198	GLY	2.1
1	A	247	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SCY	A	111[A]	9/10	0.13	-	15,17,27,29	9
1	SCY	B	111[A]	9/10	0.12	-	12,16,28,28	9
1	SCY	C	111[A]	9/10	0.15	-	13,16,29,31	9
1	SCY	D	111[A]	9/10	0.13	-	15,16,28,29	9

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1502	5/5	0.21	-	78,78,78,83	0
2	SO4	C	3501	5/5	0.16	-	49,50,51,51	0
3	CAA	D	4401	54/54	0.15	-	26,38,54,55	0
3	CAA	C	3401	54/54	0.15	-	37,47,56,57	0
2	SO4	D	4502	5/5	0.17	-	82,82,83,84	0
2	SO4	B	2501	5/5	0.16	-	44,44,46,50	0
2	SO4	C	3502	5/5	0.22	-	90,90,91,95	0
2	SO4	D	4501	5/5	0.19	-	52,53,53,56	0
3	CAA	A	1401	54/54	0.15	-	35,43,55,56	0
2	SO4	B	2502	5/5	0.23	-	81,82,82,87	0
3	CAA	B	2401	54/54	0.15	-	37,50,61,62	0
2	SO4	A	1501	5/5	0.16	-	45,47,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.